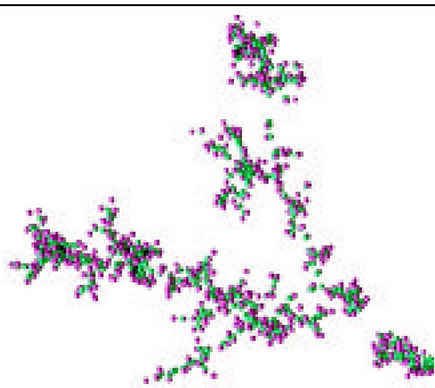
VI.G Atomistic Simulations of Radiation Damage in Metals

Introduction: High-energy neutrons, which are necessarily produced in nuclear reactors, can damage the materials used to contain the core. Not only is this a serious problem affecting the life and safety of present fission reactors, but it will present a major hurdle for future fusion reactors. The primary form of damage is atomic displacement. This occurs when energetic neutrons hit atoms in the solid, giving them enough energy to create a series, or cascade, of further displaced atoms. Under the right conditions, these displaced atoms collect at internal surfaces creating voids and causing a significant overall dimensional change. The figure to the left illustrates this swelling. It shows a comparison of originally identical samples after irradiation of one of them. Although the swelling occurs rather slowly, after large radiation doses and long times, the dimensional changes are quite extraordinary. Material scientists are using computer simulation to try to gain further insight into the detailed mechanisms of radiation damage. The goals are to predict problems over long periods of time (reactor aging) and to design new materials that are less sensitive to radiation damage.

Swelling of irradiated steel

Calculational Notes: Molecular dynamics simulations model the initial displacement of atoms caused by a single high-energy neutron. "Monte Carlo" simulation techniques model the random motion of thousands of such displaced atoms diffusing over long times. To simulate cascades requires models containing millions of interacting atoms. Gathering adequate statistics requires multiple realizations (runs).



Portion of a high-energy displacement cascade in copper

Results: The lower figure shows the results of a computer simulation of a single high-energy neutron striking a piece of copper. The small spheres represent the defects produced in the otherwise regular arrangement of atoms in the crystal structure. The green spheres represent vacant crystal lattice sites from which atoms have been displaced, and the magenta spheres represent the displaced atoms that have been pushed into places not usually occupied by atoms.

Significance: This initial work provides a detailed map of the atomic displacements. Knowing the structure is the first step to understanding the properties induced. SSI resources will permit the accumulation of thousands of events for improved statistics. It will also permit the extension to complex structural alloys, which exist in aging reactors, as well as to the development of new radiation-resistant alloys for future fission and fusion reactors. Simulation will play a particularly important role since experiments are extremely time consuming, expensive, and in some cases, impossible.